Passivated Contacts to n^+ and p^+ Silicon Based on Amorphous Silicon and Thin Dielectrics

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Abstract — Carrier recombination at the metal contact regions has now become a critical obstacle to the advancement of high efficiency diffused junction silicon solar cells. The insertion of a thin dielectric interlayer – forming a metal-insulator-semiconductor (MIS) contact – is a known approach to reduce contact recombination. However, an insulator thickness less than 25 Å is usually required for current transport, making it difficult to simultaneously achieve good surface passivation. This paper compares standard MIS contacts to a newly developed contact structure, involving hydrogenated amorphous silicon (a -Si:H) over-layers. The contact structures are trialed on both n^+ and p^+ lightly diffused surfaces, with SiO_2 and Al_2O_3 insulator layers, respectively. In both cases significant improvements in the carrier-selectivity of the contacts is achieved with the addition of the a -Si:H over-layers. Simulations of idealized cell structures are used to highlight the performance and technological benefits of these carrier-selective structures over standard locally diffused contacts.

Index Terms — amorphous silicon, silicon solar cells, selective contacts, contact passivation, high efficiency.

I. INTRODUCTION

The metal-silicon interface hosts an unavoidably large density of recombination active defects. Carrier recombination occurring at this interface places a significant limitation on the performance of devices which require high minority carrier lifetimes, such as the crystalline silicon (c -Si) solar cell. Two approaches have typically been implemented to address this issue: *i.*) the introduction of a heavily doped region immediately beneath the metal contact, and *ii.*) the reduction of the contact fraction to a smaller percentage of the cell surface area.

In the first approach, the addition of a heavy dopant concentration under the contact induces a strong asymmetry in the electron and hole concentrations, hence in their conductivities. By limiting the transport of one carrier (the minority carrier) to the metallized surface, recombination can be greatly reduced. Large reductions in metal-semiconductor contact resistivity can also be realized, as the heavier dopant concentration reduces the width of the potential barrier ubiquitous to the metal-silicon interface thereby increasing the tunneling probability for majority carriers. However, this approach is fundamentally limited by Auger recombination, which increases with increasing dopant concentration. In

addition, heavy doping also introduces detrimental effects like reduced carrier mobilities and bandgap narrowing. As such the lowest metallized recombination current parameters J_{0c} achievable by this approach are about 350 fA/cm².

The second strategy involves the reduction of the metallized region to a small percentage of the cell area – a method which is essential on the cell's sunward-side given the opacity of metals. With this reduction in contact fraction, carrier flow is constricted so that the conductance towards the metal-silicon interface is reduced [1]. Such a geometrical reduction of the conductance affects majority carriers, causing a higher resistive loss, and minority carriers, leading to a reduced recombination loss. This tradeoff of majority carrier resistance for minority carrier recombination is usually permissible given their relative influence on cell performance. However, producing cells with small contact fractions within the industrial environment has proven to be a significant technological challenge, particularly when applied in conjunction with localized heavily doped regions.

The above described fundamental and technological issues associated with metal-silicon contacts have become a roadblock for the advancement of silicon solar cells, prompting much research in the area of passivated contacts. A common approach to achieve passivation of the contacts is to physically displace the metal and silicon surfaces by the insertion of thin passivating interlayers. These contact structures are generally categorized in accordance to the electrical characteristics of the interlayer(s) as metal-insulator-semiconductor (MIS) contacts, semiconductor-insulator-semiconductor contacts, or heterocontacts.

In the context of solar cells, MIS contacts have typically utilized SiO_2 [2-4] and Al_2O_3 [5-8] for the insulators, as their thicker counterparts (>100 Å) have been successfully implemented for surface passivation in the non-contacted regions. However, the wide band-gap of these dielectrics presents large barrier heights to electrons and holes in the conduction and valence bands of c -Si. Hence, effective contacts are limited to a maximum thickness of ~25 Å in order to maintain appreciable current flow through tunneling conduction. Achieving a high level of surface passivation with a 25 Å thick dielectric (or thinner) remains a difficult task, compromising the benefit of implementing such contacts.

Fig. 1. Contact structures to be compared in this paper. Structures are referenced within the text by the names provided at the bottom. Layer thicknesses are not to scale, images represent the layer structure before annealing (after annealing *a*-Si:H and aluminum will intermix).

A proven pathway to improve the passivation quality of ultra-thin dielectric films is to apply hydrogen rich over-layers which assist in the passivation process [9, 10]. Hydrogenated amorphous silicon (*a*-Si:H) has the unique characteristics of being both an excellent hydrogen rich over-layer and being readily dissolvable in aluminum at low temperatures. With these characteristics in mind, a MIS fabrication procedure can be envisioned in which *a*-Si:H is applied on top of an ultrathin insulator to improve surface passivation, following which it is dissolved into an overlying aluminum layer by means of a low temperature anneal, resulting in the formation of a low resistance and low recombination contact [11].

To demonstrate the potential benefits of this process, this paper compares MIS contacts to n^+ and p^+ surfaces both with and without an *a*-Si:H over-layer. Ultrathin atomic-layer-deposited (ALD) Al_2O_3 and thermally grown SiO_2 insulators are used on p^+ and n^+ surfaces respectively, in line with established best passivation practices for these surfaces. The efficacy of the contacts are described by their resistive and recombination properties as quantified by the contact resistivity ρ_c and contact recombination parameter J_{0c} . Idealized cell structures are simulated to assess the potential of these different approaches and compare them to heavily doped directly metallized surfaces. The different contact structures, and their corresponding abbreviations, are given in Figure 1.

II. EXPERIMENTAL

A. Test Structure Fabrication

Accurate J_{0c} and ρ_c values cannot easily be extracted from the same test structures; therefore, pairs of test structures were prepared to be measured via photoconductive decay (PCD) and the transfer-length-method (TLM) measurements. PCD

measurements were taken on symmetrical test structures (identical layers / stacks deposited on both wafer faces) whilst TLM samples were single side only.

All samples were prepared on FZ, $>100 \text{ } \Omega\text{cm}$ resistivity, (100) oriented, p and n -type Si wafers. After saw damage etching and standard RCA cleaning, the wafers were diffused in quartz furnaces with boron (on n -type wafers) or phosphorus (on p -type wafers) so that in all cases the doping of the diffusion and substrate were opposite. Details of the final dopant profile characteristics, as determined by electrochemical capacitance voltage measurements (WEP Wafer Profiler), are given in Table I.

ALD Al_2O_3 layers were deposited at 200°C (Beneq TFS 200) using alternating cycles of trimethylaluminium and water. Purge and pulse times were chosen as to ensure a self-limiting reaction. A growth-per-cycle of $\sim 1 \text{ } \text{\AA}$ is measured for this process, extrapolated from thicker Al_2O_3 depositions. All test structures with an Al_2O_3 layer were annealed at 400°C for 15 minutes immediately prior to metallization, for surface passivation activation. SiO_2 layers were grown via rapid thermal oxidation (O_2 ambient) at 700°C in a clean quartz furnace. The *a*-Si:H layers were deposited by plasma-enhanced-chemical-vapor-deposition (PECVD) at a set temperature of either 200°C (p^+ MSIS) or 400°C (n^+ MSIS) to a thickness of $\sim 30 \text{ nm}$.

Aluminum layers were evaporated at low pressure onto samples to a thickness of $1 \text{ } \mu\text{m}$ and $\sim 10 \text{ nm}$ for the TLM and carrier lifetime test structures respectively (see Section II.B). The p^+ and n^+ MSIS structures require a further annealing step at 250°C to initiate the aluminum *a*-Si:H interaction, a more detailed explanation of the fabrication procedure of these contacts is given in [11].

Included in Table I are the directly passivated $J_{0\text{pass}}$ and directly metallized $J_{0\text{metal}}$ recombination parameters of the p^+ and n^+ surfaces. The directly passivated recombination parameters have been realized via PECVD *a*-Si:H ($\sim 30\text{nm}$) for the n^+ surface and plasma-assisted-ALD Al_2O_3 ($\sim 20\text{nm}$) for the p^+ surface, in-line with previously reported low surface recombination results on these surfaces [12, 13]. The metallized recombination parameter is measured from samples with $\sim 10 \text{ nm}$ of aluminum evaporated directly onto the diffused surfaces.

TABLE I
PHOSPHORUS AND BORON DOPANT DIFFUSION CHARACTERISTICS

Source	Sample	R_{sh} ($\Omega/\square$)	N_{surf} (cm^{-3})	$J_{0\text{metal}}$ (fAcm^{-2})	$J_{0\text{pass}}$ (fAcm^{-2})
POCl_3	n^+ MIS, n^+ MSIS	100 $\pm$ 15	3($\pm$ 1) $\times 10^{19}$	1200 $\pm$ 200	25 $\pm$ 5
	n^+ MS	20 $\pm$ 5	4($\pm$ 2) $\times 10^{20}$	350 $\pm$ 50	N/A
BBr_3	p^+ MIS, p^+ MSIS	100 $\pm$ 15	1($\pm$ 1) $\times 10^{19}$	1370 $\pm$ 200	27 $\pm$ 5
	p^+ MS	35 $\pm$ 5	2($\pm$ 2) $\times 10^{19}$	520 $\pm$ 70	N/A

* R_{sh} sheet resistance, N_{surf} surface dopant concentration, $J_{0\text{metal}}$ metallized recombination factor, $J_{0\text{pass}}$ passivated recombination factor.

Recombination parameter J_{0c} values were extracted using the Kane and Swanson technique [14] from carrier lifetime measurements taken using a photoconductive decay (PCD) instrument (Sinton WCT 120). An intrinsic carrier concentration of $n_i = 8.95 \times 10^9 \text{ cm}^{-3}$ (at 297 K) was assumed in these extractions. Only thin aluminum layers are used for these samples to ensure that sufficient light passes through the aluminum layer and that the signal from the calibrated conductance tester is not saturated by the additional conductivity of the metal.

Contact resistivity ρ_c measurements are taken using TLM measurements. The TLM contact pad patterns were photolithographically defined and isolated using an acidic Al etch. Pad spacings of 10-300 μm are used during this study. Current-voltage measurements were performed using a Keithley 2425 Source Meter (at $\sim 297 \text{ K}$) and ρ_c was extracted as per the description given in [15].

Film thicknesses were monitored by fitting reflectance data (J.A. Woolam M2000 ellipsometer) of single side polished silicon wafers deposited alongside carrier lifetime and TLM samples. Given the dependence of SiO_2 growth on the dopant concentration, the SiO_2 thickness samples were subjected to a phosphorous diffusion prior to oxidation to create an alike surface concentration.

A. Contact Characteristics

Figure 2a and b provide the ρ_c and J_{0c} dependence on SiO_2 thickness, for the n^+ contacts. Included in these plots as a reference are dotted lines indicating the position of $J_{0\text{metal}}$, $J_{0\text{pass}}$ and the directly metallized ρ_c of the diffusion profile used on the n^+ MIS and n^+ MSIS structures.

In agreement with the theoretical probability for quantum-mechanical tunneling, a strong increase in ρ_c is observed as a result of increasing insulator thickness for both the n^+ MIS and n^+ MSIS structures. Both n^+ contact structures exhibit similar resistive behavior for SiO_2 thicknesses in the 1.5 – 1.7 nm range. Above this range the n^+ MIS structure appears to maintain a lower ρ_c value than the n^+ MSIS structure, with films of 2.2 nm still achieving a ρ_c of $\sim 0.2 \Omega\text{cm}^2$.

Coupled with the increasing ρ_c is a decreasing J_{0c} , which is again seen for both contact structures. For the n^+ MSIS structures an order of magnitude reduction in recombination is obtained, as compared to $J_{0\text{metal}}$, for even the thinnest SiO_2 layers. An insulator thickness of 1.7 nm is sufficient to achieve the lower limit recombination factor of $\sim 25 \text{ fA/cm}^2$. The n^+ MIS structures show a more moderate reduction in recombination but still achieve values of $\sim 300 \text{ fA/cm}^2$ with a 1.9 nm SiO_2 layer.

Fig. 2 Contact resistivity ρ_c of a.) n^+ contacts and c.) p^+ contacts and contact recombination factor J_{0c} for b.) n^+ contacts and d.) p^+ contacts as a function of insulator thickness. Lines provide a guide to the eyes only, error bars are based off the estimated error in measurement.

An analogous set of results for the p^+ contacts as a function of the number of ALD Al_2O_3 cycles is provided in Figure 4c and d. Both p^+ MSIS and p^+ MIS structures show an increasing ρ_c trend with Al_2O_3 thickness (in this case as number of cycles), although the p^+ MSIS structure consistently achieves lower ρ_c values. The improvement in J_{oc} with Al_2O_3 thickness is not as strong as seen for the n^+ contacts – reaching at best ~ 150 fA/cm² for the p^+ MSIS structure – which is still approximately an order of magnitude lower than the corresponding J_{0metal} . Interestingly, for the p^+ MSIS structure the passivation quality seems to stop improving after 10 cycles of Al_2O_3 – producing a local minimum. The p^+ MIS structure exhibits a more gradual reduction in recombination with increasing Al_2O_3 thickness, resulting in no overlap between contact passivation and useful contact resistances. It should be noted that the ρ_c values of ~ 1 Ωcm^2 and above were extracted from contacts that deviated from pure Ohmic behavior and as such they represent a lower-limit ρ_c .

B. Significance to Solar Cells

In the context of solar cells, the efficacy of the contacts can be described by their carrier-selectivity. The carrier-selectivity of a particular region or contact structure can be generically defined as its ability to perform two separate functions: *i.*) provide a very high conductivity for one carrier type – the collected, or majority carrier; and *ii.*) present a very low conductivity to the other carrier – the minority carrier [16]. These two functions can be well represented by the parameters

ρ_c and J_{oc} , respectively. The contact resistivity ρ_c is a measure of the ability to transport majority carriers across the contact interface. A decrease in ρ_c corresponds to an increase in majority carrier conductivity. The parameter J_{oc} reflects the recombination losses occurring at the contact interface or, more generally, within the complete contact structure, which, for the structures investigated in this paper, includes the recombination in the bulk of the diffused region. The parameter J_{oc} is analogous to the conductivity presented by the contact structure towards minority carriers [17]. A very high J_{oc} means that there is minimal impediment to minority carriers flowing towards the contact, hence it means that there is a high minority carrier conductivity, and vice-versa.

An ideal contact structure should be highly selective, that is, combining very low ρ_c and very low J_{oc} . But in practice, these two properties are difficult to achieve simultaneously, and a trade-off between them needs to be found. The nature of this tradeoff is generally complicated, requiring consideration of the contact architecture. Therefore, a proper discussion of passivated contacts should also include as a third variable the fraction of the solar cell surface where the contact is implemented.

To illustrate the trade-off between ρ_c and J_{oc} , we have simulated an idealized solar cell structure with partial rear contacts (PRC) using a recently developed quasi-analytical model for such a device structure [18, 19], in conjunction with QsCell [20]. The PRC was modelled with a variable ρ_c and J_{oc} , and for each $\rho_c - J_{oc}$ combination an optimum rear contact

Fig. 3 Simulated optimum contact fraction (dotted lines) and resultant efficiency (contour plot) as a function of rear contact ρ_c and J_{oc} . Results presented in this work are superimposed over the contour plot.

fraction (dashed lines) is found and the resultant efficiency calculated. Figure 6 presents the results of the simulations. A list of assumptions and values used in the simulation are provided in Table II. Note that we have assumed an homogeneous dopant diffusion on the rear surface, that is, a p^{++} device structure. Such a diffusion helps to transport carriers laterally towards the local contacts, but its presence does not dramatically change the results of the simulations, particularly for larger contact fractions. The results in Fig. 6 are consistent with recent simulations of a similar nature [21].

Fig. 3 shows that there is a relatively broad parameter space in which a high efficiency can be achieved. A low ρ_c permits to afford relatively high J_{0c} , as long as the contact fraction is very small. As an example, the optimized n^{++} MS and p^{++} MS contacts introduced in Figure 1 and Table I are shown on this plot as a blue and orange diamonds respectively. Such a solar cell with localized diffused contacts, frequently referred to as PERL cell, has led to conversion efficiencies up to 25% (note that the efficiency in Fig. 3 is only 24.5% because we have assumed a relatively low photogenerated current density of 40 mA/cm²).

TABLE II
SIMULATION ASSUMPTIONS AND VALUES

Symbol	Parameter	Assumption / value
J_{0front}	Front recombination factor	1 fA/cm ²
J_{0rear}	Rear recombination factor (in non-contacted area)	1 fA/cm ²
R_{sh_front}	Front diffusion sheet resistance	120 $\Omega/\square$
R_{sh_rear}	Rear diffusion sheet resistance	100 $\Omega/\square$
	Bulk type, resistivity	n-type, 1 Ωcm
W	Wafer thickness	160 μm
J_g	Generation current density	40 mA/cm ²
τ_{bulk}	Bulk lifetime	Richter intrinsic lifetime [22]

On the other extreme, it is possible to also achieve a high efficiency even if ρ_c is relatively high, as long as J_{0c} is very small and the contact fraction is high. Although strictly not applicable to this plot, the position of standard silicon heterojunction (SHJ) contacts, with a J_{0c} of 5 fA/cm² and a ρ_c of 0.3 Ωcm^2 , also sits at $\sim 25\%$ in line with best results for these structures.

To show the significance of the n^{+} and p^{+} passivated contacts presented in this paper, their corresponding $J_{0c} - \rho_c$ trends are superimposed over the simulated contour plot.

For the n^{+} MIS contacts the highest efficiencies are seen for the thinnest SiO₂ interlayers, which should be applied in small contact fractions. The addition of the a -Si:H over-layer in the n^{+} MSIS clearly improves the selectivity of the contact – mostly due to a reduction in the minority carrier conductivity (reduction in J_{0c}). n^{+} MSIS contacts with an oxide layer of ~ 1.65 nm produce the optimum tradeoff between J_{0c} and ρ_c with idealized efficiencies of over 25%. A significant advantage of this $J_{0c} - \rho_c$ combination, as compared to the

n^{++} MS localized diffusion approach, is that large contact fractions (10 – 30%) are permissible – potentially simplifying the fabrication procedure.

As mentioned in Section III.B, the p^{+} MIS contact characteristics exhibit no benefit over the corresponding directly metallized case. The addition of the a -Si:H over-layer in the p^{+} MSIS structure is again seen to result in strong improvements in the contact-selectivity. With ~ 5 cycles of ALD Al₂O₃, the p^{+} MSIS contact characteristics produce a slightly lower, but similar, idealized cell efficiency to the localized p^{++} MS contacts. Benefits in terms of fabrication simplicity, due to the removal of the local diffusion step, could prove sufficient to outweigh this difference.

V. CONCLUSION

This paper has explored the benefits of a newly developed carrier-selective contact, whose fabrication procedure utilizes an a -Si:H capping step for MIS contact formation. Passivated contact structures both with (MSIS) and without (MIS) the additional a -Si:H over-layer have been trialed on lightly diffused $p^{+}/\text{Al}_2\text{O}_3$ and n^{+}/SiO_2 structures. These were also compared to optimized n^{++} and p^{++} metal-silicon contacts. The results of the investigation have shown a significant enhancement in carrier-selectivity as a result of the additional a -Si:H capping step for both the n^{+} and p^{+} contacts.

Simulated idealized solar cell structures show that for the n^{+} MSIS contacts an optimum configuration with a SiO₂ layer of ~ 1.65 nm produces efficiencies over 25%. These simulations suggest that the n^{+} MSIS contacts can be applied to large area fractions of the rear surface, and hence offer advantages over the traditional localized heavy diffusion approach, both in terms of performance and process simplicity.

The p^{+} MSIS contacts revealed poorer $J_{0c} - \rho_c$ combinations, with corresponding lower idealized efficiencies, but may still offer advantages over the p^{++} MS contact in terms of process simplicity.

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